Estimating RVE sizes for 2D/3D viscoplastic composite materials

Kamel Madi[1], Samuel Forest[1], Dominique Jeulin[2] and Michel Boussuge[1]

(1) Centre des Matériaux - UMR CNRS 7633, Ecole des Mines de Paris, B.P. 87, 91003 Evry, France
(2) Centre des Matériaux - Centre de Morphologie Mathématique - UMR CNRS 7633, Ecole des Mines de Paris, B.P. 87, 91003 Evry, France

1 Introduction

This work aims to study the representativity of the measurements obtained from a limited domain of the random viscoplastic two–phase material and to precise the statistical definition of the Representative Volume Element (RVE).

2 Numerical tools for homogenization problems

The computational methods used in this work introduce explicitely the 2D/3D morphology of the considered random heterogeneous materials. A generic representation of the microstructure of random materials is chosen, namely the so–called Voronoï mosaics. The finite element method is chosen for the 2D/3D computations presented in this work. The corresponding parameters used in the finite element simulations of the creep behavior of a two–phase aggregate are given: mesh size, constitutive equations of the constituents and boundary conditions.

2.1 Generic representation of the microstructure

A good candidate to generate random media is the Voronoï mosaic model since it provides a granular representation of the microstructure and since it introduces a random character in the phase distribution (Torquato, 2002). It is an ideal representation of isotropic random polycrystals (Gilbert, 1962; Barbe et al., 2001). The Voronoï mosaic model reproduces a random distribution of grains in space according to a Poisson process, building a Voronoï tesselation of space (Gilbert, 1962). It is also possible to superimpose a constraint of periodicity at the boundary of the volume in the generation of the Voronoï mosaic as proposed in (Decker and Jeulin, 2000) and used in (Kanit et al., 2003). One must distinguish the 2D case to the 3D one. These two models are different. Moreover, one can precise that 2D slices generated by a 2D Voronoï mosaic model cannot be obtained from 2D slices of a volume built following a 3D Voronoï mosaic model. For the 2D case (resp. 3D), the number of grains N_S (resp. N_V) is given by the relation $S_G N_S = S$ (resp. $V_G N_V = V$), where S_G (resp. V_G) is the mean surface of a grain (resp. mean volume of a grain) and S (resp. V) the surface (resp. volume) of the grains. As no intrinsic length scale is introduced in our simulations, absolute values of grain sizes are not required. The convention is made that the mean surface of one 2D Voronoï cell (resp. the mean volume of one 3D Voronoï cell), S_G (resp. V_G), is 1. As a result, a surface (resp. volulme) contains in average $N_S = S$ (resp. $N_V = V$) Voronoï cells.

Figures 1a (resp. 1c) show a realization of a 2D (resp. 3D) Voronoï mosaic obtained by the algorithm proposed in (Barbe et al., 2001). Each color corresponds to a different grain. The phases (hard and soft) are then distributed randomly among the various grains according to a given volume fraction, which leads to the distribution shown in figure 1b (resp. 1d). In the present study, we have chosen a volume fraction of 70% for the hard phase (the hard phase is called P_1) and 30% for the soft phase (the soft phase is called P_2).

2.2 Constitutive equations

The constitutive equations adopted for modelling the response of the phases are based on a standard elastoviscoplastic framework. The total strain is decomposed into elastic and plastic parts and Hooke's law is

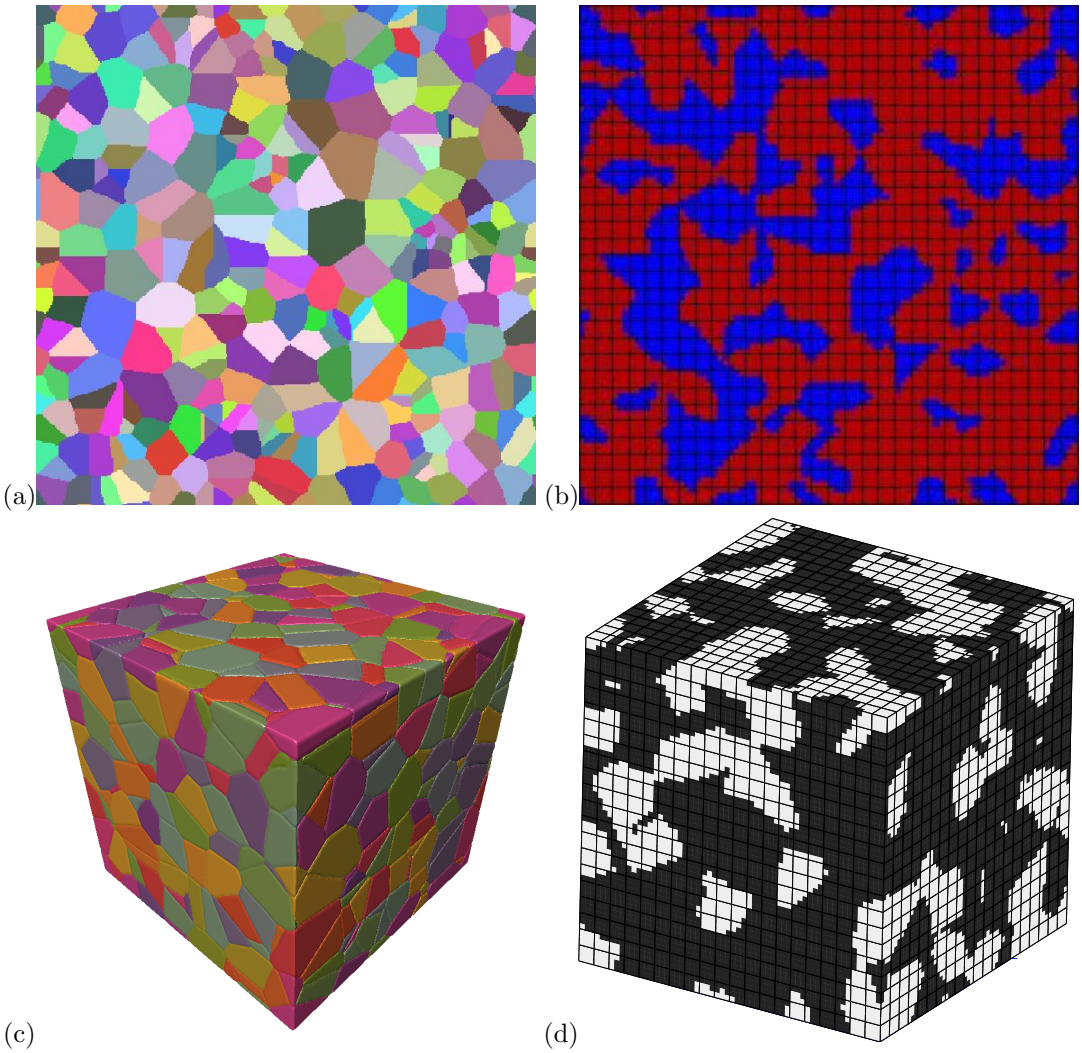


Figure 1: (a) 2D microstructure (Voronoï mosaic containing 300 grains), (b) Meshing of a Two-phase material: 2D Voronoï mosaics containing 300 grains with 70% of phase1 and 30% of phase2, (c) 3D microstructure (Voronoï mosaic containing 470 grains), (d) Meshing of a Two-phase material: 3D Voronoï mosaics containing 470 grains with 70% of phase1 and 30% of phase2.

Phase	Volume Fraction (%)	n	K $(MPa^{1/n})$	E (GPa)	ν
Hard phase	70	3.5	5000	441	0.25
Soft phase	30	4	950	307	0.25

Table 1: Volume fraction and mechanical data for the two phases. K and n are parameters in the power law used for the viscoplastic behavior of the two phases.

adopted:

$$\varepsilon_{ij} = \varepsilon^e_{ij} + \varepsilon^p_{ij}, \quad \sigma_{ij} = c_{ijkl}\varepsilon^e_{kl} \tag{1}$$

For simplicity, the creep law introduced for both phases is a simple power law without hardening:

$$\dot{\varepsilon}^p_{ij} = \dot{p}\frac{3}{2}\frac{s_{ij}}{J_2(\sigma_{ij})}, \quad \dot{p} = \left(\frac{J_2(\sigma_{ij})}{K}\right)^n, \quad J_2(\sigma_{ij}) = \sqrt{\frac{3}{2}s_{ij}s_{ij}} \tag{2}$$

J_2 denotes the second invariant of the stress tensor and is also called the von Mises equivalent stress. The deviatoric part of the stress tensor is s_{ij} and p is the cumulative equivalent viscoplastic strain. The materials properties of each phase are thus defined by the two parameters: K and n. These parameters are given in Table 1.

2.3 Finite element meshing

The finite element mesh associated with the image of the microstructure is obtained using the so–called multi-phase element technique (Lippmann et al., 1997; Barbe et al., 2001). A regular 2D (resp. 3D) finite element grid is superimposed on one image of the Voronoï mosaics. The material property is attributed to each integration point according to the color of the nearest pixel (resp. voxel) of the image. As a result, two phases may be present inside some elements. Figure 1b (resp. 1d) shows such a mesh for a 2D (resp. 3D) microstructure and the distribution of both phases. The elements are quadratic squares (8 nodes) (resp. quadratic bricks (20 nodes)) with complete integration (9 Gauss points) (resp. (27 Gauss points)).

The appropriate mesh density, defined as the average number of elements required for ensuring a given accuracy in the results of the numerical simulations, must be first determined in 2D and 3D. For that purpose, a specific 2D (resp. 3D) microstructure made of 100 grains is used, with a volume fraction equal to 70% of phase P_1 and 30% of phase P_2. Shear creep tests were simulated by applying a constant macroscopic shear stress Σ_{12} equal to 10 MPa, with the boundary conditions as explained in section 2.5. The number of cells and the geometry of the microstructure are unchanged but different mesh resolutions are used. The number of finite elements was changed from 100 to 8000 elements.

The results given in figure 2 show the convergence of the macroscopic shear $\dot{E}_{12}$ of the aggregate as a function of the number of elements. In 2D, a mesh density of 20 quadratic elements per grain is necessary to get a precision of 1% on the mean strain rate. In 3D and with the same precision, 17 quadratic elements per grain are necessary. We verified that this mesh density leads to a convergence of the local stress and strain fields with a precision better than 5%.

2.4 Ensemble average

The computation cost limits the possible number of grains that can be handled in the simulation of one volume element V. In particular, such a limit size may be smaller than a so–called Representative Volume Element of the material (Kanit et al., 2003). In this case, the properties that can be computed are not necessarily the desired effective properties but merely apparent properties of the investigated volume.

In (Huet, 1990; Hazanov and Huet, 1994), Huet derive relationships between apparent physical properties obtained on a large elastic specimen (not necessarily a RVE) and on a set of smaller ones obtained as a uniform partition of the considered large specimen. One of the conclusions is that the effective properties are bounded by the ensemble average of results obtained on the set of smaller specimens:

$$\overline{\underset{\sim}{\mathbf{C}}^{app}_{SUBC}} \leq \underset{\sim}{\mathbf{C}}^{eff} \leq \overline{\underset{\sim}{\mathbf{C}}^{app}_{KUBC}} \tag{3}$$

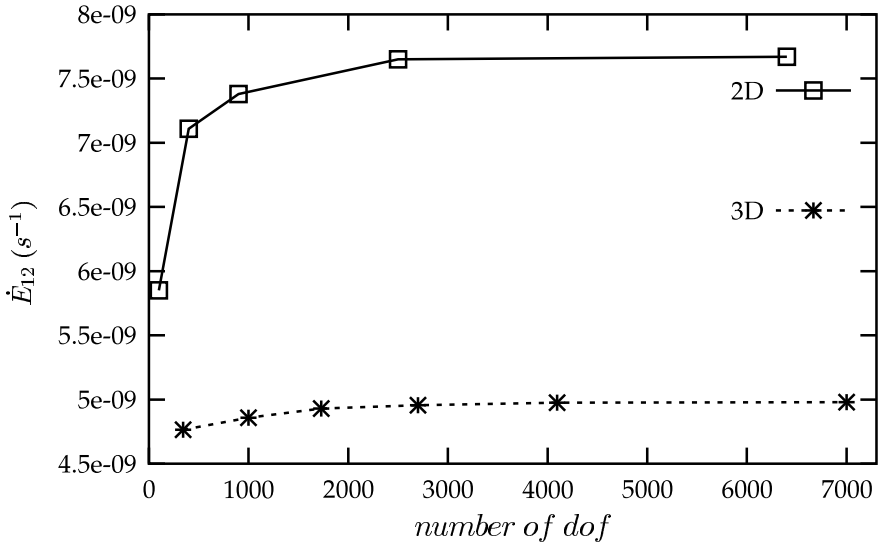


Figure 2: Evolution of $\dot{E}_{12}$ as a function of the number of elements (2D/3D). Creep tests were performed under periodic boundary conditions for a macroscopic shear stress $\Sigma_{12} = 10\ MPa$.

where:

$\overline{\underset{\approx}{\mathbf{C}}^{app}_{SUBC}}$ is the ensemble average of apparent modulus tensor obtained with Static uniform boundary conditions (SUBC) on a partition of V.

$\overline{\underset{\approx}{\mathbf{C}}^{app}_{KUBC}}$ is the ensemble average of apparent modulus tensor obtained with Kinematic uniform boundary conditions (KUBC) on a partition of V.

$\underset{\approx}{\mathbf{C}}^{eff}$ is the effective modulus tensor of the representative volume element. The inequality 3 has to be integrated in terms of quadratic forms.

When the large specimen is a RVE, the effective properties found with both SUBC and KUBC are the same. Recently, Kanit et al. (Kanit et al., 2003) show that one can estimate the effective properties of heterogeneous elastic materials by computing and ensemble averaging the apparent properties of a sufficient number of volumes containing a given number of grains. This statistical approach is extended in the present work to the nonlinear case.

2.5 Boundary conditions

The notations used within the context of the mechanics of heterogeneous materials are the following (Suquet, 1997): the local strain and stress fields inside the considered volume elements are denoted by $\varepsilon_{ij}(x_k)$ and $\sigma_{ij}(x_k)$. The macroscopic strain and stress tensors are then defined as the corresponding average values over each considered volume:

$$E_{ij} =< \varepsilon_{ij} >= \frac{1}{V}\int_V \varepsilon_{ij}, dV, \quad \Sigma_{ij} =< \sigma_{ij} > \tag{4}$$

In order to invesigate the creep behavior of the heterogeneous material, one must be able to prescribe a given macroscopic stress tensor Σ_{ij} to each considered volume element V. For that purpose, several types of boundary conditions are available. They are listed and compared in the reference (Kanit et al., 2003).

The boundary conditions that lead to the smallest boundary layer effects and therefore to smaller representative volume elements are the periodicity conditions. The displacement field over the entire volume then reads:

$$u_i = E_{ij}x_j + v_j \quad \forall x_i \in V \tag{5}$$

where E_{ij} is the prescribed macroscopic strain tensor. The fluctutation v_i is periodic: it takes the same values at two homologous points on opposite faces. The traction vector $\sigma_{ij}n_j$ takes opposite values at two homologous points on opposite faces of V. The numerical resolution of this problem within the finite element

context is such that the dual forces associated to E_{ij} are the components of the macroscopic stress tensor Σ_{ij} (Besson et al., 2001). Consequently, the periodicity conditions can be used either for prescribing mean strain or mean stress components.

In the present work, all the simulations were performed by applying a constant macroscopic shear stress Σ_{12} during the creep tests, the remaining stress components being set to zero. The macrocospic stress tensor, Σ_{ij}, takes this form:

$$\Sigma_{ij} = \begin{pmatrix} 0 & \Sigma_{12} & 0 \\ \Sigma_{12} & 0 & 0 \\ 0 & 0 & \end{pmatrix} \tag{6}$$

Therefore, the macroscopic strain rate of the aggregate is equal to the macroscopic viscoplastic strain rate:

$$< \dot{\varepsilon}_{ij} >=< \dot{\varepsilon}^e_{ij} > + < \dot{\varepsilon}^v_{ij} >, \quad \dot{E}_{ij} = \dot{E}^e_{ij} + \dot{E}^v_{ij} \tag{7}$$

so:

$$\dot{E}^e_{ij} = 0, \quad \dot{E}_{ij} = \dot{E}^v_{ij} \tag{8}$$

2.6 Apparent viscoplastic properties

The problem is to define this notion of apparent property for viscoplasticity. In this case, the strain energy takes this form:

$$\dot{e} \hat{=} < \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\dot{\boldsymbol{\varepsilon}}} >= \underset{\sim}{\boldsymbol{\Sigma}} :< \underset{\sim}{\dot{\boldsymbol{\varepsilon}}} >= \underset{\sim}{\boldsymbol{\Sigma}} : \underset{\sim}{\dot{\boldsymbol{E}}} \tag{9}$$

where $\underset{\sim}{\dot{\boldsymbol{E}}}$ and $\underset{\sim}{\boldsymbol{\Sigma}}$ are the macroscopic strain and stress tensors. Shear creep tests being performed and assuming that a stationary stress state has been reached, one can write:

$$\underset{\sim}{\boldsymbol{\Sigma}} :< \underset{\sim}{\dot{\boldsymbol{\varepsilon}}} >= \underset{\sim}{\boldsymbol{\Sigma}} : \underset{\sim}{\dot{\boldsymbol{E}}}^v, \quad 2\Sigma_{12} < \dot{\varepsilon}_{12} >= 2\Sigma_{12}\dot{E}^v_{12}, \quad < \dot{\varepsilon}_{12} >= \dot{E}^v_{12} \tag{10}$$

We make the hypothesis that the macroscopic strain rate of the 2D/3D aggregates can be also approximated by a simple creep law. It is known that, in general, this assumption is not verified, except when both phases have the same parameter n (Rougier et al., 1993), but we suppose that it is only suitable under certain conditions: shear creep tests in a precise domain of stresses ($\leq$ 30 MPa) at 1400K. Two parameters n^{app}, K^{app} are then identified such that:

$$\dot{E}^v_{ij} = \dot{p}\frac{3}{2}\frac{S_{ij}}{J_2(\Sigma_{ij})}, \quad \dot{p} = \left(\frac{J_2(\Sigma_{ij})}{K^{app}}\right)^{n^{app}}, \quad J_2(\Sigma_{ij}) = \sqrt{\frac{3}{2}S_{ij}S_{ij}} \tag{11}$$

J_2 and S_{ij} are the second invariant and the deviatoric part of the macroscopic stress tensor.

Then, taking into account relation 11, relation 10 become:

$$2 < \dot{\varepsilon_{12}} >= \sqrt{3}^{n^{app}+1}\Sigma_{12}^{n^{app}}\frac{1}{{K^{app}}^{n^{app}}}, \quad \frac{1}{{K^{app}}^{n^{app}}} = \frac{2 < \dot{\varepsilon_{12}} >}{\sqrt{3}^{n^{app}+1}{\Sigma_{12}}^{n^{app}}} \tag{12}$$

We define an apparent property for viscoplasticity $P_v = P_v^{app}$ as:

$$P_v^{app} = \frac{2 < \dot{\varepsilon_{12}} >}{\sqrt{3}^{n^{app}+1}{\Sigma_{12}}^{n^{app}}} \hat{=} \frac{1}{{K^{app}}^{n^{app}}} \tag{13}$$

The procedure of determination of P_v^{app} is the following. For each domain size (2D/3D), shear creep tests were performed under periodic boundary conditions on each realization at 10 MPa. The contrast between strain rates of both phases under a shear stress of 10 MPa is 35. For a given domain size and for each realization, the average shear strain rate $\dot{E}_{12} =< \dot{\varepsilon_{12}} >$ is computed; n^{app} and K^{app} are calibrated using a numerical identification from the ensemble average obtained on shear creep tests performed on each realization at two different stress levels (10 and 30 MPa). One can now compute for each realization the apparent property for viscoplasticity P_v^{app}.

3 Statistical definition of the size of the RVE

We have seen in section 2.4 that the apparent properties are defined from spatial average of additive fields $\varepsilon_{12}^{\cdot}$ over a surface S (resp. volume V). We will consider now fluctuations of the average values over different realizations of the random composite material inside the surface S (resp. volume V). The variance of the apparent properties for each domain size is used for the determination of the RVE.

A good way to have a convenient measurement of the size of a RVE of a stationary and ergodic random structure is the notion of integral range (Matheron, 1971; Matheron, 1975; Lantuejoul, 1991; Cailletaud et al., 1994; Jeulin, 2001). It is a range which gives information on the domain size of the microstructure for which the parameters measured in this volume have a good statistical representativity. This notion is very useful to predict the variability of the properties of a material. This notion of integral range has already been introduced by T. Kanit (Kanit et al., 2003) and this work is an extension of this notion to the nonlinear case.

Considering P_v as an ergodic stationary function, one can compute the variance $D^2_{P_v}(S)$ (resp. $D^2_{P_v}(V)$) of its average value $\overline{P_v}$ over the surface S (resp. volume V) (Matheron, 1971; Lantuejoul, 1991):

$$D^2_{P_v}(S) = \frac{D^2_{P_v} A_2}{S}, \quad (D^2_{P_v}(V) = \frac{D^2_{P_v} A_3}{V}) \tag{14}$$

where $D^2_{P_v}$ is the point variance of P_v and A_2 (resp. A_3) is the integral range of the random function P_v. The scaling law 14 is valid for an additive combination of the variable P_v over the region of interest S (resp. V), when its size is such that: $S > A_2$ (resp. $V > A_3$). In the case of a two-phase viscoplastic composite material with creep properties (n_1,K_1) for phase 1 (volume fraction $P_1 = P$) and (n_2,K_2) for phase 2 (volume fraction $P_2 = 1 - P$), the point variance $D^2_{P_v}$ of random variable P_v over the surface S (resp. volume V) is given by:

$$D^2_{P_v} = \overline{P_v^2} - \overline{P_v}^2, \quad D^2_{P_v} = P(1-P)(P_{v_1} - P_{v_2})^2 \tag{15}$$

Using relation 13, one can write:

$$D^2_{P_v} = P(1-P)[\frac{1}{K_1^{n_1}} - \frac{1}{K_2^{n_2}}]^2 \tag{16}$$

Regarding the material as a random taking of independant realizations, the size of the RVE, based on statistical arguments, must be considered as a function of parameters: the physical property of interest, the contrast of properties, the volume fraction of components and the number of realizations of the microstructure (Kanit et al., 2003). In the statistical theory of samples that can be found for instance in (Kreyszig, 1988; Kanit et al., 2003), the absolute error ϵ_{abs} and relative error ϵ_{rel} on the mean value of the studied property P_v, obtained with n independent configurations of surface S (resp. volume V), is a function of the variance $D_{P_v}(S)$ (resp. $D_{P_v}(V)$) by:

$$\epsilon_{abs} = \frac{2D_{P_v}(S)}{\sqrt{n}}, (\epsilon_{abs} = \frac{2D_{P_v}(V)}{\sqrt{n}}) \quad \epsilon_{rel} = \frac{\epsilon_{abs}}{\overline{P_v}} \tag{17}$$

Taking into account relation 14, one can write:

$$S = \frac{4D^2_{P_v} A_2}{\epsilon^2_{rel} P_v^2 n}, (V = \frac{4D^2_{P_v} A_3}{\epsilon^2_{rel} P_v^2 n}) \tag{18}$$

The size of the Representative Surface Element RSE (resp. Representative Volume Element) can therefore be estimated as the surface (resp. volume) for which for instance n=1 realization is necessary to estimate the mean property P_v with a relative error ϵ_{rel}=1%. One can decide also to operate on smaller volumes and to consider n realizations to obtain the same relative error.

S (number of grains)	300	833	1400	2000
n (number of realizations)	1000	300	300	300
mean value $\overline{\dot{E}_{12}}$(x$10^9 s^{-1}$)	8.26	8.10	8.10	8.09
mean value $\overline{P_v}$(x10^{13})	2.63	2.58	2.59	2.58
variance $2D_{P_v}$(x10^{14})	6.78	3.84	3.28	2.52
ϵ_{rela}	0.8%	0.8%	0.8%	0.6%

Table 2: Dispersion and mean value of the apparent property for viscoplasticity P_v^{app} as a function of the domaine size S.

V (number of grains)	96	150	470	715	1000
n (number of realizations)	112	66	81	25	11
mean value $\overline{\dot{E}_{12}}$(x$10^9 s^{-1}$)	5.85	5.60	5.56	5.65	5.65
mean value $\overline{P_v}$(x10^{13})	2.56	2.45	2.44	2.47	2.47
variance $2D_{P_v}$(x10^{14})	10.5	6.41	4.51	3.28	2
ϵ_{rela}	3.8%	3.2%	2.1%	2.7%	2.4%

Table 3: Dispersion and mean value of the apparent property for viscoplasticity P_v^{app} as a function of the domain size V.

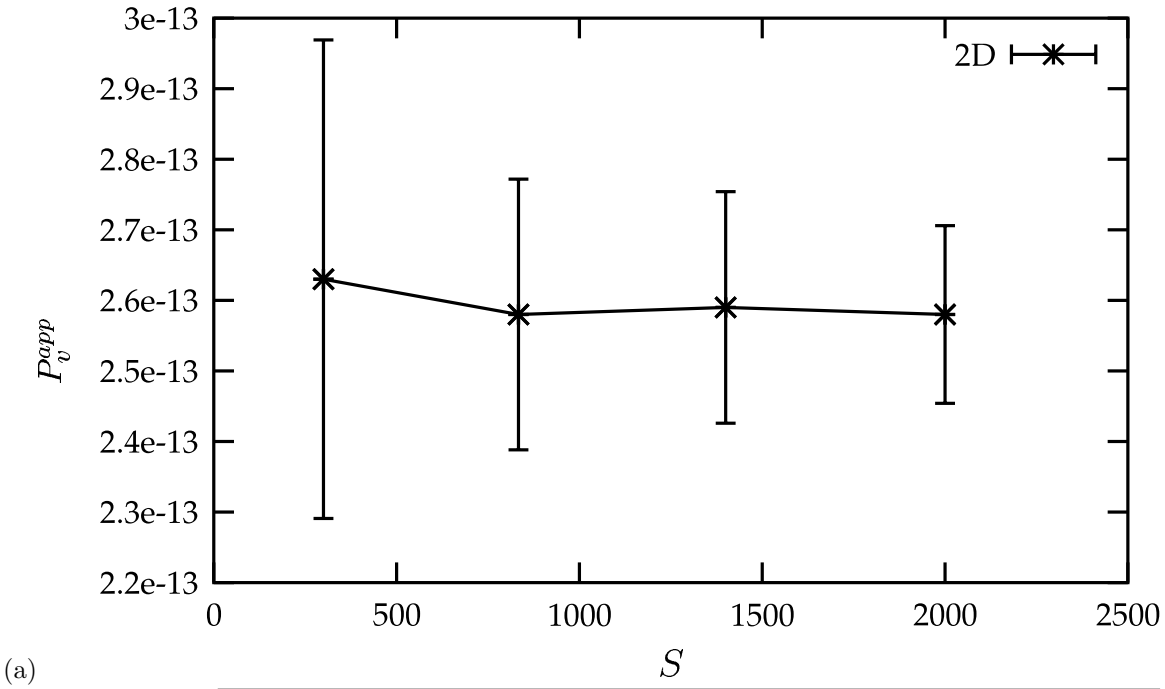
4 Results

4.1 2D/3D Fluctuations of the effective property

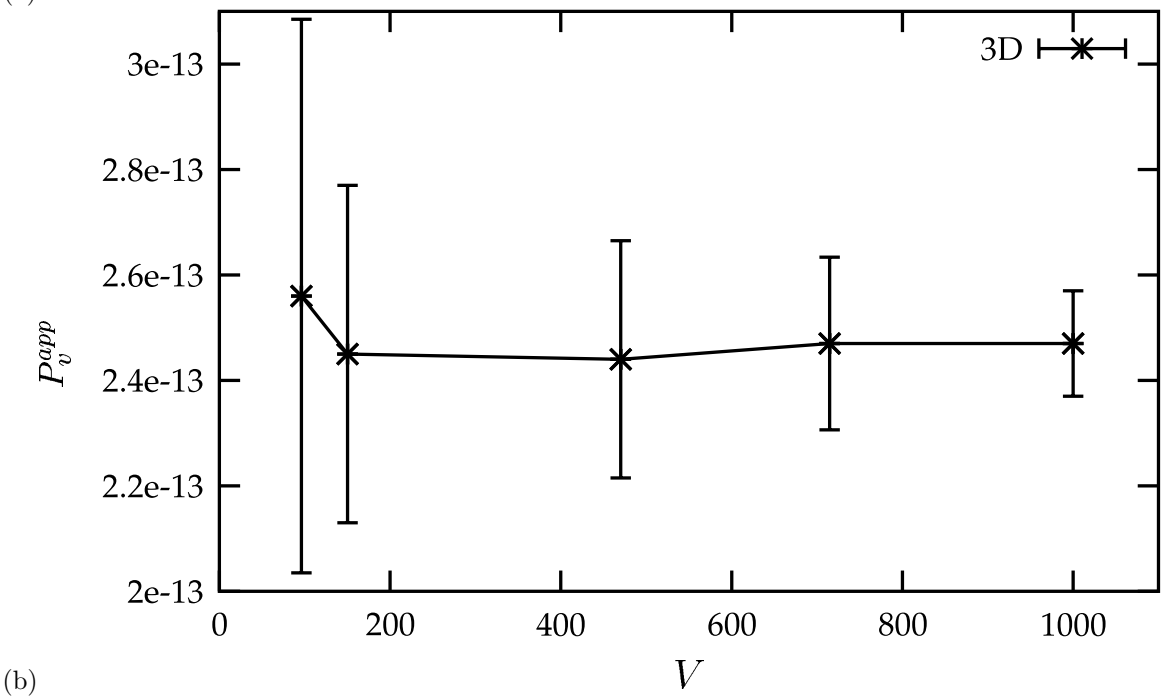
The number of grains and realizations considered in our 2D (resp. 3D) simulations are reported in table 2 (resp. table 3). The obtained mean values $\overline{P_v}$ and dispersions $2D_{P_v}$ of the apparent property for viscoplasticity P_v^{app} are given, in 2D (resp. 3D), in figure 3a (resp. figure 3b), as a function of the domain size. Values are reported in tables 2 and 3.

It is observed, for both 2D and 3D domains, that the dispersion of the results decreases when the size of the domain increases and that the mean values converge towards the same limit for large domains, which is the wanted effective property. One can see in tables 2 and 3 that the values of the effective property for viscoplasticity P_v^{eff} are practically the same in 2D and 3D. The relative error between both values is lower than 4%. Moreover, one can oberve that a bias is found in the mean value for small volume sizes. This bias is well-known (Huet, 1990; Sab, 1992). Even using periodic boundary conditions, the mean value computed on small aggregates cannot represent the effective response of the two-phase material. In 2D, from a surface containing 800 grains and, in 3D, from a surface containing 150 grains, the mean value does not depend on the size of the domain.

Finally, we can compare the 2D and 3D dispersions obtained. First, one can precise that the number of grains in 2D, N_S, is different to the one in 3D, N_V. N_S is obtained simply from N_V by the relation: $N_S = N_V^{\frac{2}{3}}$. In 3D, the maximum number of grains considered in our simulations is 1000, which corresponds to about 100 grains in 2D. If we compare the dispersion obtained in 3D for the volume containing 1000 grains with the ones obtained in 2D (figure 3, see also tables 2 and 3), we can conclude that the 2D dispersion is greater than the 3D one.



(a)



(b)

Figure 3: Dispersion and mean value of the apparent property for viscoplasticity P_v^{app}, as a function of the domain size: (a) 2D, (b) 3D. Periodic boundary conditions are considered.

Property	Integral Range A_2	α
P_v $(P = 70\%, \frac{\dot{\varepsilon}_1}{\dot{\varepsilon}_2} = 35)$	1.3	1
Volume fraction $(P = 70\%)$	1.018 (Gilbert, 1962)	1
Property	Integral Range A_3	α
P_v $(P = 70\%, \frac{\dot{\varepsilon}_1}{\dot{\varepsilon}_2} = 35)$	0.63	1
P_v $(P = 70\%, \frac{\dot{\varepsilon}_1}{\dot{\varepsilon}_2} = 35)$	1.19	1.1
P_v $(P = 70\%, \frac{\dot{\varepsilon}_1}{\dot{\varepsilon}_2} = 35)$	2.18	1.2
Volume fraction $(P = 70\%)$	1.111 (Kanit et al., 2003)	1
	1.179 (Gilbert, 1962)	1
κ $(P = 70\%, \frac{E_1}{E_2} = 100)$	1.02 (Kanit et al., 2003)	0.78
μ $(P = 70\%, \frac{E_1}{E_2} = 100)$	1.322 (Kanit et al., 2003)	0.763
λ $(P = 70\%, \frac{\lambda_1}{\lambda_2} = 100)$	2.619 (Kanit et al., 2003)	1.033

Table 4: Values of the integral range A_2, A_3 and the coefficient α for the apparent property for viscoplasticity P_v^{app} and for other linear properties.

4.2 2D/3D Computations of the Integral Range

Starting from relations (14), one can identify A_2 and A_3 from the simulations performed. We propose to test a power law according to the relation:

$$D^2_{P_v}(S) = D_{P_v^2}(\frac{A_2}{S})^{\alpha}, \quad (D^2_{P_v}(V) = D_{P_v^2}(\frac{A_3}{V})^{\alpha}) \tag{19}$$

α equal to 1 means that the model is well fitted. Equation (19) can be written:

$$log(D^2_{P_v}(S)) = -\alpha log(S) + (log(D_{P_v^2}) + \alpha log(A_2)), \quad (log(D^2_{P_v}(V)) = -\alpha log(V) + (log(D_{P_v^2}) + \alpha log(A_3))) \tag{20}$$

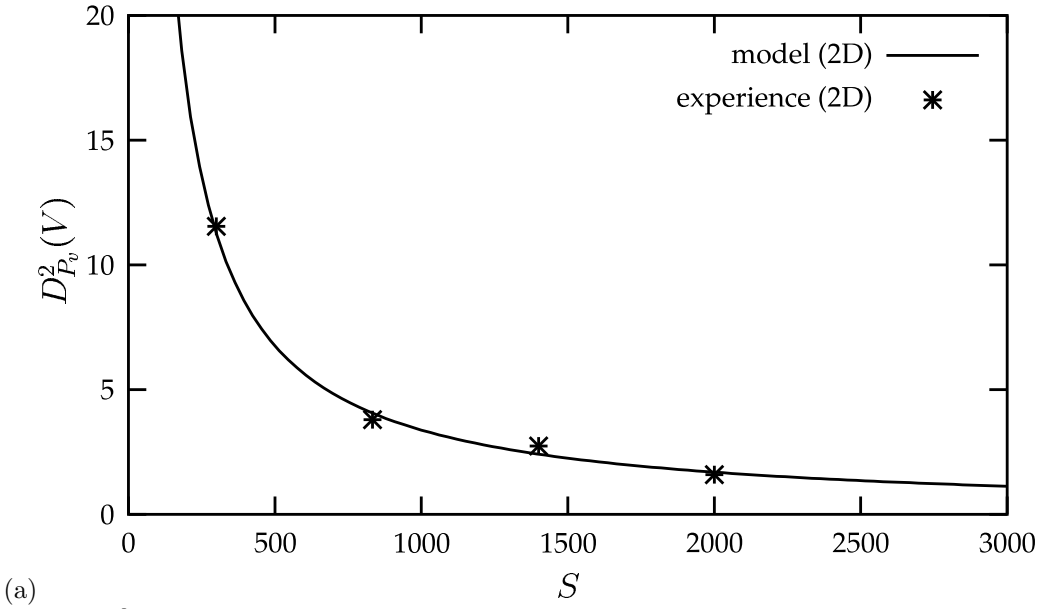
Our data were fit to relation (20) for the apparent property for viscoplasticity P_v^{app}. The obtained A_2, A_3 and α parameters are reported in table 4.

The quality of the fitting can be seen in figure 4 where the variances of simulated results and the model are compared. One can see that the model is well fit in 2D with A_2 equal to 1.3 and α equal to 1. In 3D, the fitting is less perfect with A_3 equal to 1.19 and α equal to 1.1. We have tested the sensibility of the parameter A_3 to a slight variation of α. Results are reported in table 4 and show that A_3 varies between 0.63 and 2.18 when α is comprised in the interval [1;1.2]. It is shown in figure 4b that the quality of the fitting is improved and more acceptable for α equal to 1. A possible explanation of a better fitting in 2D compared to 3D is probably the size of the domains considered. The maximum number of grains in 2D is 2000. The maximum number of grains in 3D is 1000, which corresponds only to about 100 grains in 2D. Then, larger volumes (or more realizations ?) should be used to possibly improve the quality of the fitting and to precise correctly the value of A_3 (more closed to 0.63 than to 1.19). Finally, it seems that A_3 (closed to 0.63) is lower than A_2 (1.3). It means that the variance seems to decrease twice slower, with the size of the domain, in 2D than in to 3D. This is in agreement with the previous result stating that the 2D dispersion of the property P_v is greater than the 3D one.

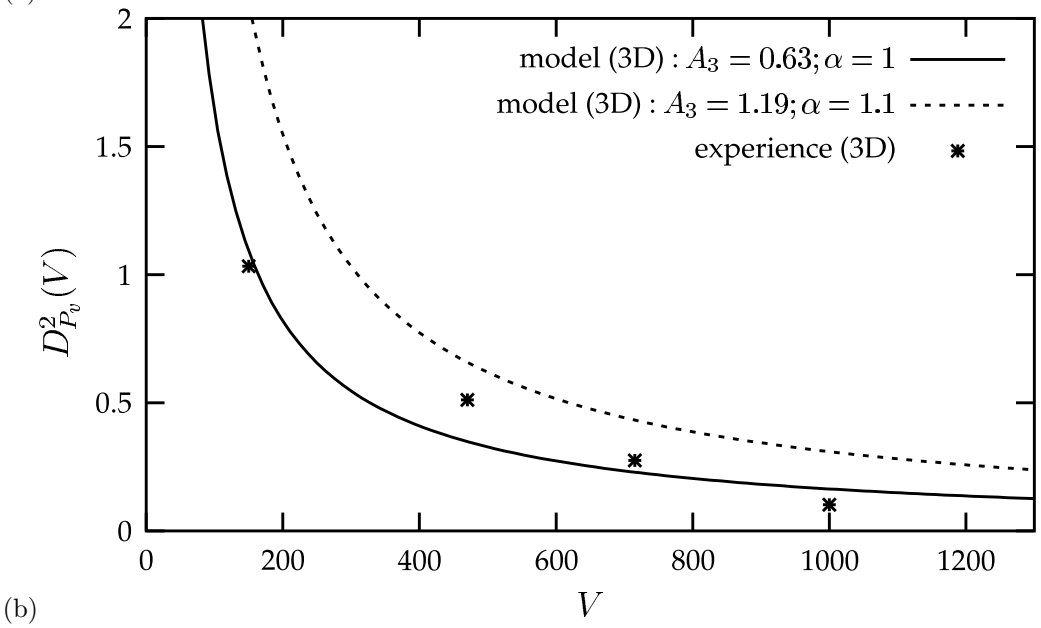
5 Discussion

5.1 Comparison with other properties

The values of the integral ranges obtained in 2D and 3D are closed to 1. We can see in table 4 that A_2 (1.3) and A_3 (closed to 0.63) are practically in the same order of the integral range of the volume fraction predicted by both theory (Gilbert, 1962) and numerical simulations of a two-phase voronoï mosaic (Kanit



(a)



(b)

Figure 4: Variance of the apparent property for viscoplasticity P_v as a function of the domain size: simulations and model, (a) 2D ($\alpha = 1$; $A_2 = 1.3$) , (b) 3D (α = 1-1.1; A_3 = 0.63-1.19)

Relative precision	ϵ_{rel}=1%	ϵ_{rel}=5%	ϵ_{rel}=10%
$S^{2D}_{P_v}$ (n=10 realizations)	20311	831	203
$S^{2D}_{P_v}$ (n=300 realizations)	677	27	7
$V^{3D}_{P_v}$ (n=10 realizations)	10739 ($S^{3D->2D}$ = 502)	429 ($S^{3D->2D}$ = 58)	105 ($S^{3D->2D}$ = 22)
$V^{3D}_{P_v}$ (n=300 realizations)	357	14	4
V^{3D}_{κ} (n=10 realizations)	13340	533	133
V^{3D}_{κ} (n=300 realizations)	444	17	5
V^{3D}_{μ} (n=10 realizations)	71253	2806	701
V^{3D}_{μ} (n=300 realizations)	2339	93	23

Table 5: Minimimal sizes of the RSE and RVE determined for nonlinear and linear properties, for a given precision ϵ_{rel} and a given number of realizations n.

et al., 2003). We can also compare our results with values of integral range obtained in 3D with other linear properties (see table 4) using periodic boundary conditions, with the same volume fraction (P = 70%) but different contrasts between the properties of the constituents (Kanit et al., 2003). Results are also reported in table 4. The contrast in shear modulus μ is high (120), whereas the contrast in bulk modulus κ is lower (5). The value obtained for the integral range of the nonlinear property P_v in 3D (A_3 closed to 0.63) is always lower than the ones obtained for the bulk κ, shear μ moduli and for the thermal conductivity λ. It means that the variance decreases more slowly with the size of the domain in the linear case than in the nonlinear case.

5.2 Determination of the size of the Representative Volume Element

Using relations 18, one can now estimate the minimal sizes of the RSE and the RVE for a given relative error ϵ_{rel} and a given number n of realizations. Results are reported in table 5. 3D results are compared with the ones obtained for linear properties presented in section 4.2.

When ϵ_{rel}=1% and for n=10 realizations, it is shown that one must take about $S^{2D}_{P_v}$ = 20311 and $V^{3D}_{P_v}$ = 10739 for the apparent property for viscoplasticity P^{app}_v. Or, $V^{3D}_{P_v}$ = 10739 grains in 3D corresponds to about $S^{3D->2D}_{P_v}$=500 grains in 2D ($N_S = N_V^{\frac{2}{3}}$). $S^{2D}_{P_v}$ is 40 times greater than $S^{3D}_{P_v}$ when ϵ_{rel}=1% and 10 times when ϵ_{rel}=10%.

Comparing our results with other linear properties, one can see that:

- $V^{3D}_{P_v}$ is practically equal to V^{3D}_{κ}, whereas the contrast chosen in our simulations is 35 and the contrast between bulk moduli is 5,
- $V^{3D}_{P_v}$ is 7 times lower than V^{3D}_{μ}, wheras the contrast chosen in our simulations is 35 and the contrast between shear moduli is 120

Then, the size of the Representative Volume Element (RVE) seems to be smaller in the nonlinear case than in the linear case, for the present study.

6 Conclusions and prospects

This work aimed to estimate RVE sizes for 2D/3D viscoplastic composite material. The microstructure was representated by Voronoï mosaics. An apparent property for viscoplasticity P_v was proposed with its numerical procedure of determination. 2D/3D computations were performed under periodic boundary conditions to estimate the fluctuations of the effective property P^{eff}_v and to compute the integral range. Results show that the 2D dispersion is greater than the 3D one. A_3 (closed to 0.63) is smaller than A_2 (1.3), which means that the variance seems to decrease twice slower, with the size of the domain, in 2D than in to 3D. We found that the integral range A_3 obtained for P_v is always lower than the ones obtained for

other linear properties, like the bulk κ, shear μ moduli and the thermal conductivity λ. It means that the variance decreases more slowly with the size of the domain in the linear case than in the nonlinear case. Computations of RVE sizes show that:

- the size of the RVE in 2D is larger than the size of the RVE in 3D,
- the size of the RVE seems to be smaller in the nonlinear case than in the linear case.

References

Barbe, F., Decker, L., Jeulin, D., and Cailletaud, G. (2001). Intergranular and intragranular behavior of polycrystalline aggregates. Part 1: FE model. *International Journal of Plasticity*, 17:513–536.

Besson, J., Cailletaud, G., Chaboche, J.-L., and Forest, S. (2001). *Mécanique non linéaire des matériaux*. 445 p., Hermès, France.

Cailletaud, G., Jeulin, D., and Rolland, P. (1994). Size effect on elastic properties of random composites. *Engineering computations*, 11:99–110.

Decker, L. and Jeulin, D. (2000). Simulation 3D de matériaux aléatoires polycristallins. *Revue de Métallurgie-CIT/Science et Génie des Matériaux*, février 2000:271–275.

Gilbert, E. N. (1962). Random subdivisions of space into crystals. *Ann. Math. Stat.*, 33:958–972.

Hazanov, S. and Huet, C. (1994). Order relationships for boundary conditions effect in heterogeneous bodies smaller than the representative volume. *J. Mech. Phys. Solids*, 42:1995–2011.

Huet, C. (1990). Application of variational concepts to size effects in elastic heterogeneous bodies. *J. Mech. Phys. Solids*, 38:813–841.

Jeulin, D. (2001). *Caractérisation Morphologique et Modèles de Structures Aléatoires*. Extrait de: Homogénéisation en mécanique des matériaux 1, Hermès.

Kanit, T., Forest, S., Galliet, I., Mounoury, V., and Jeulin, D. (2003). Determination of the size of the representative volume element for random composites : statistical and numerical approach. *International Journal of Solids and Structures*, 40:3647–3679.

Kreyszig, E. (1988). *Advanced engineering mathematics*. Wiley International Edition, New York.

Lantuejoul, C. (1991). Ergodicity and integral range. *Journal of Microscopy*, 161:387–403.

Lippmann, N., Steinkopf, T., Schmauder, S., and Gumbsch, P. (1997). 3d-finite-element-modelling of microstructures with the method of multiphase elements. *Computational Materials Science*, 9:28–35.

Matheron, G. (1971). *The theory of regionalized variables and its applications*. Paris School of Mines publications.

Matheron, G. (1975). *Random sets and integral geometry*. J. Wiley, New York.

Rougier, Y., Stolz, C., and Zaoui, A. (1993). Représentation spectrale en viscoélasticité linéaire des matériaux hétérogènes. *Comptes Rendus de l'Académie des Sciences Série II*, 316:1517–1522.

Sab, K. (1992). On the homogenization and the simulation of random materials. *Eur. J. Mech. Solids*, 11:585–607.

Suquet, P. (1997). *Continuum micromechanics*. CISM Courses and Lectures No. 377, Springer Verlag, Berlin.

Torquato, S. (2002). *Random Heterogeneous Materials*. Springer.